

Subsurface Uncertainties and Technology Limitations

The following 27 uncertainty headings were developed using Chapter 4 of the document, “*Uncertain Predictions of Contaminant Behavior at INEEL: A Roadmap for Addressing Current Limitations through Vadose Zone Studies, INEEL/EXT-2001-552-Draft Rev 0, September, 2001*”. The complete document can be found at www.inel.gov/environment/water in the INEEL Vadose Zone Science and Technology Section Roadmap - 2002 section of the webpage by clicking on Project Reports. Additional uncertainties were added and modifications made to the original uncertainties during an uncertainties verification meeting held March 21, 2002. The uncertainties are broken down into four areas:

- Predicting Physical Transport
- Transformation Processes: Geochemical and Microbial
- Simulating and Estimating Contaminant Source Terms
- Monitoring, Characterization, Instrumentation, and Data Analysis

Predicting Physical Transport:

- 1) **Available field data are of insufficient quality and quantity for use in predictive simulation.**

Translation: Much of the available field data are insufficient in most cases for model calibration because of insufficient frequency, density, quality and quantity. Available data are often sporadic or extremely low level detections that are uncertain. Because of these data problems, confidence in the data is low and they are determined to be unsuitable to use for model calibration, which is necessary before attempting predictive simulations.

- 2) **Conceptual Models are often inadequate for prediction because they do not incorporate necessary physical and biogeochemical processes.**

Translation: Models are still highly simplistic and often fail to capture the complex interplay of physical, chemical and microbial processes in the subsurface. Such processes could be mobilizing, immobilizing or having no effect on contaminant movement. The simplicity of the models results from a lack of data to characterize the complex mechanisms and/or a lack of understanding of the mechanisms. For example, in the case of carbon tetrachloride at the RWMC, the impact of microbial degradation is unknown.

- 3) **Nonlinear governing equations for multiphase flow requires iterative solution schemes. (technical limitation)**

Translation: This is a technology limitation. The computer simulations for vadose zone flow and transport solve non-linear governing equations, which require iterative solution schemes. As a result computer simulation times are often in the range of hours to weeks. Thus simple conceptual models are chosen to cut down the computer simulation time. Resulting in simple representations of the subsurface heterogeneity and geochemical properties. As well as simplifying

assumptions such as steady state flow to address transient events such as episodic recharge and deterministic assessments when probabilistic assessments are needed...

4) Various sources of uncertainty and their relative impact on the predictability of transport is unknown and currently unqualified.

Translation: No quantitative method has been developed for assessing the uncertainty of any given prediction—to take into account problems with data quality and sparsity, as well as the simplicity of the model itself. Methods of dealing with uncertainty similar to those developed for seismic hazards assessment are needed in order to determine how much confidence we should have in the modeling results.

5) Knowledge of stratigraphic and structural controls on flow patterns in the vadose zone and the aquifer is limited.

Translation: Available geologic data are insufficient and too sparse to determine geologic controls for most of the site area outside of the facility areas.

6) Limited information is available on possible vertical transport in the aquifer.

Translation: Geologic and monitoring well data are limited and are insufficient to determine the amount of vertical water movement in the aquifer.

7) Flow direction and temporal behavior in the aquifer is limited.

Translation: Available field and monitoring well data are insufficient at the depth of the aquifer to determine local flow direction and temporal behavior. This is due to insufficient well density and insufficient well depth (most wells just sample the very top of the aquifer).

8) Little is known about the effects of hydrothermal variations on flow and transport in the aquifer.

Translation: Temperature data suggest that input of geothermal heat and water into the aquifer from depth is variable across the INEEL area. The effects on aquifer flow (velocity and direction) and groundwater chemistry are largely unknown.

Transformation Processes: Geochemical and Microbial:

9) Mechanisms and parameters describing adsorption of contaminants onto INEEL materials have not been adequately developed or measured.

Translation: The values used in models to describe the amount of a given contaminant that can be expected to be absorbed by the subsurface material it is passing through over time are estimates.

10) Conditions leading to facilitated transport are unknown.

Translation: We are unable to identify the conditions that facilitate contaminant transport in the vadose zone. For example, ultra-small particles called colloids may adsorb contaminants and stay suspended in water, possibly contributing to contaminant migration. While chemical components can adsorb onto immobile solid particles of the rock matrix, they also can adsorb onto these small colloidal particles that can be carried along with the flowing liquid phase. We don't completely understand the likelihood of contaminants to take the form of more than one phase or to form colloids. The phase of the contaminant directly affects its potential to migrate through the subsurface.

11) Microbial effects on contaminant degradation transport rates, and mechanisms in both the vadose zone and the aquifer have not been addressed.

Translation: Contaminants in the subsurface are affected by microbial populations. Accurate mathematical descriptions for these interactions do not exist. We do not completely understand the interactions between microbes and the various contaminants in the subsurface, as well as the rate and extent of biological changes. To date, we have collected insufficient data to allow meaningful conclusions to be drawn about microbial effects on contaminant transport rates in the vadose zone and the aquifer.

Simulating and Estimating Contaminant Source Terms

12) Near-field hydraulic conditions and their influence on contaminant release and migration are unknown.

Translation: The properties of the subsurface around a leaking containment vessel (such as a tank) will not reflect the properties of the surrounding area because this 'near-field' area was disturbed when the waste container was originally placed. The hydrology and vapor transport characteristics of this area will be different than the surrounding area. Water flow in this area is generally treated as a uniform process with the surrounding area although it is more likely that fluid flow is non-uniform and episodically event driven.

13) Chemistry of the near-field environment (e.g. the oxidation-reduction potential and solubility effects) may significantly affect the release and the rate of migration.

Translation: The chemistry of the near-field may significantly affect the rate of contaminant migration and this has not been factored into *in situ* waste treatment planning. For example, grouting mechanically stabilizes the waste but can also cause a significant alteration of the chemical environment for contaminant release. Solution chemistry refers to chemicals dissolved in liquid. Redox refers to oxidation-reduction potential of a chemical—which is a measure of chemical oxidation. Chemical oxidation helps to control how reactive (how likely to change and what it will react with) the chemical is in the subsurface environment.

14) Temporal behavior of the containers and waste forms relative to contaminant release is unknown.

Translation: This uncertainty has two parts, 1) container failure and 2) release rates of contaminants to the environment, for transport in the subsurface. Of particular concern for container failure is the corrosion rates of metal containers. Of particular concern for releases to the environment are release rates due to corrosion of activated metals, leaching of contaminants from infiltrating water, and diffusion of volatile contaminants (organics, H-3, C-14) from failed or partially failed containers. We have little data on container failure processes and contaminant release from failed containers. Vapor release from failed containers occurs (in the vadose zone) but has not been quantified. Measurements we take today may not reflect what we see next year or ten years from now. We must understand the physical and chemical processes in order to understand the data.

15) Conceptual model of flow within the source material

Translation: Current models treat water flow through the near field material around the contaminants or source terms as a steady flow. However, the flow is more likely to be sporadic and non-uniform. In other words, there may be large flows as one large event and long periods of no flow through the near field materials. Field analytical methods are needed to be able to evaluate the effects of these types of flow conditions.

16) Contaminant Inventory Uncertainties

Translation: Estimates of contaminant inventories have significant uncertainties in both historical accidental release areas and disposals whose contents were not carefully recorded. Determining the extent of the contamination requires boring into the soil and burial sites, a potentially hazardous and expensive process that also brings contaminated materials to the surface. Release rates from a failed containment system are not measurable, and have to be estimated. Overall spill magnitude often has to be estimated as well. Existing invasive and non-invasive characterization methods have difficulty simulating and estimating the effects of different contaminant sources.

17) The extent to which interactions between phases (vapor, liquid, organic interactions, etc.) affects transport is unknown.

Translation: Little data are available on how mixed phases (i.e. liquid and vapor) move through the vadoze zone or what reactions take place when different phases are mixed together.

18) Contaminant source terms (history and magnitude) are not currently quantifiable.

Translation: Simulating and estimating the effects of different contaminant sources is complicated by several factors. Determining the extent of the contamination requires boring into the soil, a potentially hazardous and expensive process that also brings contaminated materials to the surface. Release rates from

a failed containment system are not measurable, and have to be estimated. Overall spill magnitude often has to be estimated as well.

Monitoring, Characterization, Instrumentation, and Data Analysis:

- 19) Temporally varying fluid saturations and pressures, precipitation, evapotranspiration, temperature, barometric pressure, etc., are collected sporadically.**

Translation: As a result of a wide range of ongoing activities, properties such as soil pH, pressure, temperature, saturation, biological activity, oxidation, etc. are measured sporadically (both in terms of where, when and how often they are sampled), despite a direct interrelationship to weather changes, seasonal water flux, etc. Since short duration episodic events may affect infiltration and transport of contaminants, this results in data that has little or questionable value for predictive modeling purposes because there may be no data during the primary event. This complicates both remediation and modeling efforts. In other words, our monitoring campaigns have been of short duration, and have not coincided with important episodic events (such as flooding), so we know very little about the physical and chemical changes in the subsurface due to such events.

- 20) Spatially variable parameters have been measured for a very small percentage of the total volume of the geomedium existing in the INEEL subsurface.**

Translation: Through a wide of range of activities, various parts of INEEL's subsurface have been only partially characterized. The subsurface is highly variable both on spatial and time scales. Large variability exists in structure, water saturation, hydrologic properties, composition, etc.

- 21) Relationships between extracted concentrations, small volume measurements of vadose zone parameters, biologic indicators, and state variables to those of the larger subsurface environment are unknown.**

Translation: It's difficult to determine how useful any subset of measurements are without comparing them to a comprehensive set of measurements. In a highly variable subsurface environment such as the INEEL's, variables such as fluid flow rates, soil pH, microbial populations, etc. can change dramatically from one location to another. The techniques to obtain these variables are not currently available. Using current technology, we are unable to comprehensively measure what is happening in the subsurface. We do not have a comprehensive data set for comparison.

- 22) Preferred pathways are not detected or monitored, and there is relatively little information available.**

Translation: INEEL's subsurface basalt layers have not been comprehensively characterized. Fracture characteristics such as orientation, length, density and

aperture have not been quantified. Small scale preferred pathways are generally not important but preferred pathways on the facility scale need to be identified.

23) Instrument bias and accuracy are often unknown.

Translation: The effects of installing instrumentation in the subsurface are still largely unquantifiable, and potential changes in instrument response with time are unknown. The accuracy of instrument readings is difficult to assess, and readings are often not comparable from one location to another.

24) Quantifying the relative contributions to non-ideal behavior will require advances in detection and discriminatory analysis capabilities.

Translation: Poorly understood physical and chemical processes at the pore or other small scales may have significant effects on the flow and transport at the field scale. This is a basic science uncertainty that needs to be addressed in order to improve our predictions of flow and transport. Because our understanding of the subsurface environment is incomplete, we base our investigations around an ‘ideal’ set of assumptions based on our current understanding. We cannot verify the assumptions because instruments and methodologies are not available to measure at small scales (such as flow in a fracture or fluid movement at a fracture-matrix interface).

25) Laboratory-determined properties have not been related to field-scale values and conditions.

Translation: Laboratory scale experiments are generally not large enough to mimic the full complexity of geo/hydro/bio/chemical processes that occur in the real world subsurface. Because of this, data derived from laboratory research is instructive to some degree, but of limited practical application. We can’t simply take laboratory observations, scale them up and then explain observations in the field—laboratory data is too simplistic and limited in scope.

26) Geophysical logs and the tools for analyzing basalt logs are inadequate for conceptual model development.

Translation: Due to drilling methods and geophysical tools used at present and in the past on the INEEL, it is difficult to obtain physical and hydrologic parameters for the rocks and to correlate geophysical logs with the actual geology present.

27) The extent of well construction affects on vadose zone and aquifer monitoring results is unknown.

Translation: Data are insufficient to determine what changes in flow patterns and transport is caused by placing a monitoring well in the hydrostatic regime. Also, it is unknown what chemical changes are taking place near the monitoring well due to reactions of the groundwater with the well materials due to corrosion.